NATIONAL ENERGY RESEARCH SCIENTIFIC COMPUTING CENTER

Simulation Can Explain – *and Help Avoid* – Radiation Damage in Ceramics

Objective: **Simulation aimed at atomic-level understanding of structural defects in materials subjected to extreme conditions.**

Implications: **Radiation tolerant ceramics are needed for nuclear waste immobilization. This work examined processes that can result in degradation of thermo-mechanical properties and reduced chemical durability.**

Accomplishments: **Simulations have shed light on radiation damage and defect accumulation in silicon carbide, zircon, zirconia, uranium dioxide and pyrochlores.**

- **Identified amorphization mechanisms.**
- **Demonstrated that ceramics can be designed to dissipate radiation damage or self anneal leaving the material undamaged.**

NERSC: **Used *DL_POLY* code on Franklin, Jacquard, 256-512 cores**

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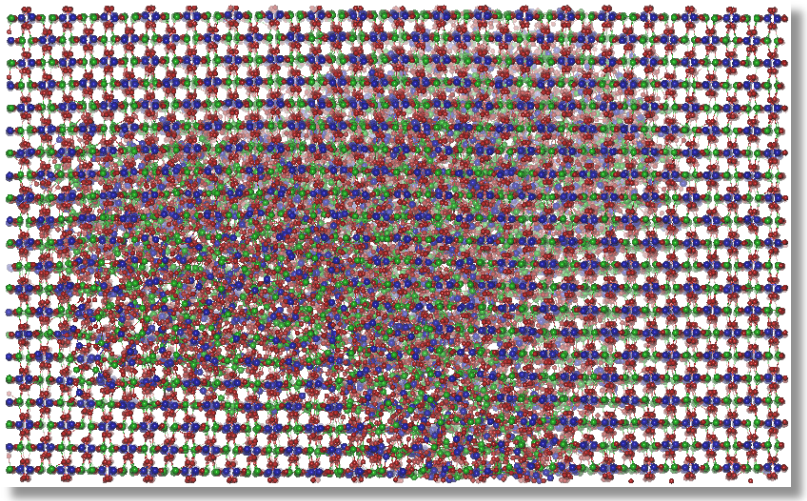

Result of a molecular dynamics simulation of Zircon ($ZrSiO_4$) showing damage to the crystal lattice as a result of high-energy uranium recoil. The simulation revealed the occurrence of direct-impact amorphization of this otherwise durable mineral.

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